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ISOLATED CO LINES FOR USE IN COMBUSTION GAS DIAGNOSTICS

ENGINE TEST FACILITY
ARNOLD ENGINEERING DEVELOPMENT CENTER
AIR FORCE SYSTEMS COMMAND
ARNOLD AIR FORCE STATION, TENNESSEE 37389

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Prepared for

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High resolution ($\simeq$ 0.1 cm^{-1}) measurements of both emission and absorption spectra in the fundamental band of CO (from 2,000 to 2,200 cm^{-1}) have been made of a variety of samples representing a wide range of temperatures and pressures using a Fourier transform spectrometer. Examination of these spectra have indicated the presence of a number of isolated CO lines that appear potentially useful for determination of CO concentration and temperature in

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20. ABSTRACT (Continued)

combustion gas flows. The spectra are analyzed and the isolated lines identified.

PREFACE

The work reported herein was conducted by the Arnold Engineering Development Center (AEDC), Air Force Systems Command (AFSC), under Program Element 65807F. The results of the research were obtained by ARO, Inc., AEDC Division (a Sverdrup Corporation Company), operating contractor for the AEDC, AFSC, Arnold Air Force Station, Tennessee, under ARO Project Number R32S-06A. The authors of this report are B. Krakow, E. L. Kiech, and H. A. McAdoo, ARO, Inc. Dr. Herman E. Scott is the Air Force project manager. The manuscript (ARO Control No. ARO-ETF-TR-76-86) was submitted for publication on August 6, 1976.

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1.0 INTRODUCTION

A technique for in situ analysis of carbon monoxide (CO) in combustion gas systems is needed at AEDC. Infrared analysis is peculiarly well suited to the CO molecule since it has a fairly strong fundamental band consisting of well spaced vibration-rotation lines in the spectral range from 2, 000 to 2, 200 wavenumbers (Ref. 1). For reduction of infrared data, it is desirable to have measurements of isolated CO lines.

The fundamental infrared CO band is flanked by carbon dioxide (CO_2) and water vapor (H_2O) bands. The wavelength ranges of the CO_2 and H_2O bands expand at high temperatures, increasing the tendency of these bands to overlap and interfere with CO lines. Since the concentrations of CO_2 and H_2O are usually much larger than CO in combustion gases, even the weaker lines of these molecules can have substantial intensity relative to CO lines. Some CO lines can also overlap each other. In principle, the overlapping of these lines does not preclude their use in CO analysis, but it makes calculations more difficult.

In order to find and specify isolated CO lines that would be useful for combustion gas diagnostics, CO spectra have been studied in both emission and absorption in a variety of samples. The experiments are described in Section 2, the resulting spectra are presented in Section 3, and isolated lines for use in combustion gas diagnostics are specified in Section 4 of this report.

2.0 EXPERIMENTAL APPARATUS

High resolution measurements of CO spectra of several samples of interest have been made with an EOCOM high resolution Fourier transform spectrometer (FTS) model 7101, which is a Michelson interferometer (Ref. 2) with appropriate position-monitoring and data-recording equipment. This interferometer was used in a frequency range from 1, 800 to 3, 700 wavenumbers with an indium antimonide (InSb) detector and a calcium fluoride (CaF_2) beamsplitter. The maximum resolution is 0. 07 cm^{-1}. The spectral measurements included both laboratory and test cell sources. In both cases, samples of substantially different temperatures were observed.

2.1 LABORATORY SETUP

In the laboratory, an F/6 beam of radiation emitted or transmitted by small samples was collected by an 8-in. cassegrain telescope which transmitted it to the interferometer as a 2-in. collimated beam. The 1-mm interferometer detector was focused to a 2.6-mm spot by the 8-in. telescope. For transmittance measurements, a Globar® was focused on this spot in a matching F/6 beam by a 6-in. cassegrain telescope.

Flames or absorption cells were placed at the telescope focus for studies in emission or absorption, respectively. Figure 1 pictures the laboratory setup with a 10-cm absorption cell in the optical beam of the interferometer-spectrometer.

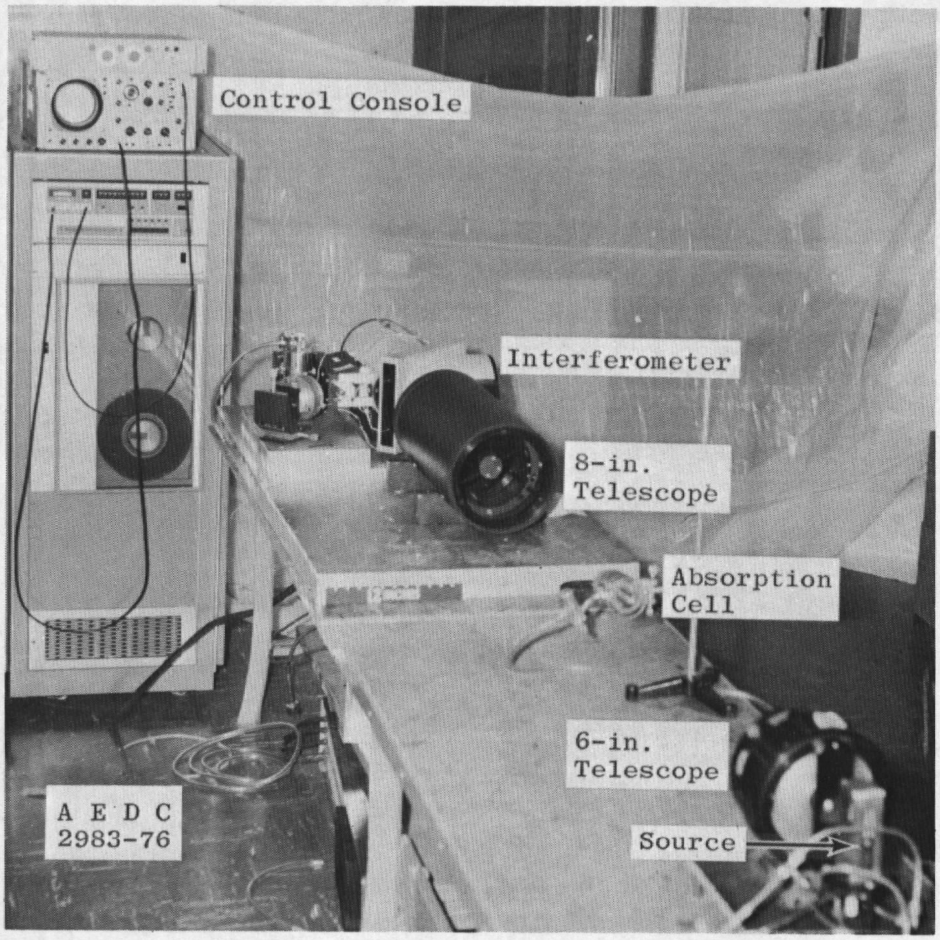

Figure 1. Photograph of laboratory apparatus used to obtain high resolution measurements of CO emission and absorption spectra.

2.2 TEST CELL MEASUREMENTS SETUP

High resolution spectra of rocket plumes were obtained in two test cells (T-3 and R-2H) at AEDC (Ref. 3).

In measurements in the T-3 test cell, the interferometer-spectrometer was one of eight optical instruments which were aligned so that their fields of view passed through a point on the centerline of the test cell (Fig. 2). Both 500- and 1,000-lbf liquid propellant rocket engines burning nitrogen tetroxide/monomethylhydrazine (N_2O_4/MMH) were used in this test. Various oxygen-to-fuel (O/F) ratios and nozzle configurations were used during the tests at simulated altitudes greater than 100,000 ft. The interferometer viewed the plume at an elevation angle of 24 deg through a calcium fluoride window in the test cell wall. The instrument had a 0.15-deg field of view and a 3-in.-diam aperture at the cell centerline. The background was a liquid nitrogen-cooled black panel.

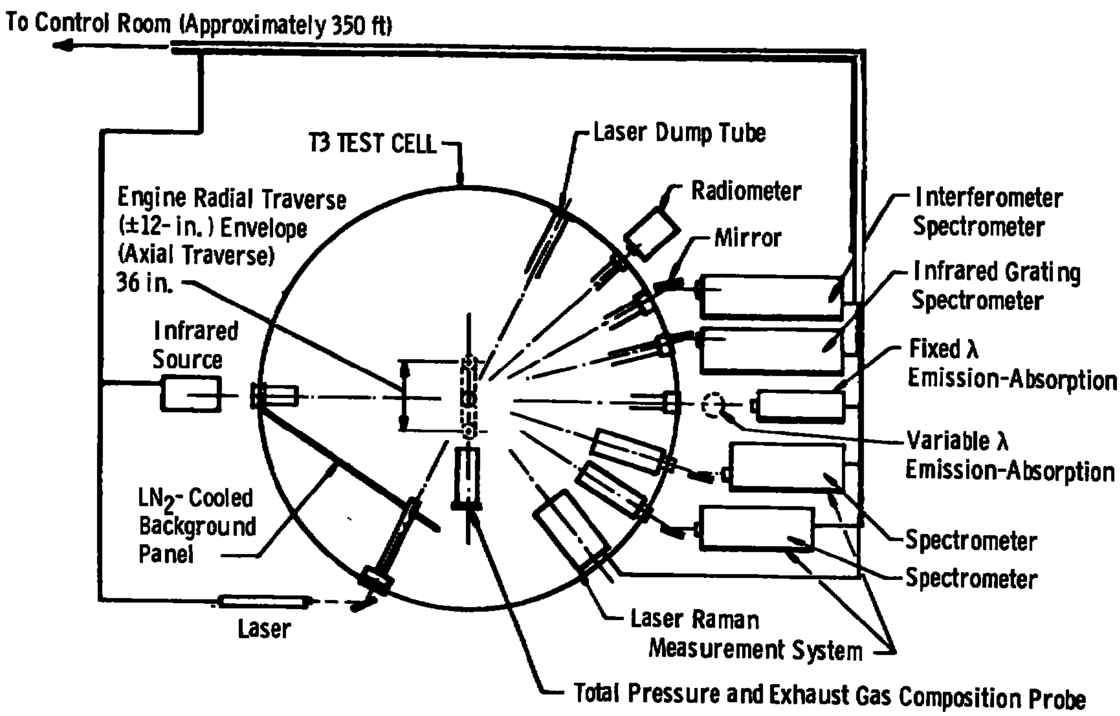

Figure 2. Arrangement for high resolution spectral radiation measurements from rocket plume in Test Cell T-3.

In the R-2H test cell, the interferometer-spectrometer was one of seven optical instruments which were aligned so that their fields of view passed through the centerline of the test cell (Fig. 3). The engine used in this test was a 5-lbf thrust rocket burning N_2O_4/MMH at various O/F ratios. The interferometer viewed the plume on a horizontal line of sight through a calcium fluoride window in the test cell wall. The instrument had a 0.15-deg field of view and a 2.2-in. aperture at the cell centerline. A liquid nitrogen-cooled black panel was inserted in the cell near the wall opposite the interferometer window to minimize background interference when the interferometer was used. This panel blocked the line of sight of the UV-visible spectrometer (Fig. 3), which was not used at the same time as the interferometer. Parameters of both model rocket engines used are shown in Table 1.

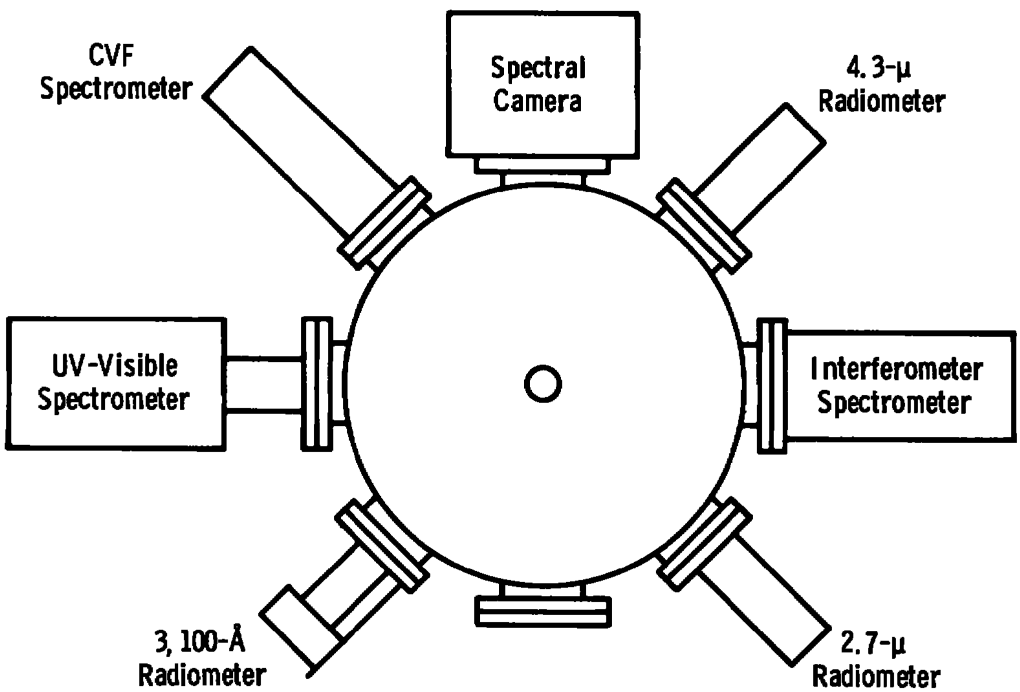

Figure 3. Arrangement for high resolution spectral radiation measurements from rocket plume in Test Cell R-2H.

Table 1. Rocket Engine Parameters

Parameter	Test Cell T-3	Test Cell R-2H
Thrust	1, 000 lb	5 lb
Chamber Pressure	500 psia	50 psia
Propellants	N_2O_4/MMH	N_2O_4/MMH
Nozzle Geometry	Conical	Conical
Nozzle Area Ratio	25	40
Nozzle Exit Diameter	6 in.	1.55 in.
Oxygen to Fuel Ratio (O/F)	1.82	1.59

3.0 RESULTS

CO spectra in the IR fundamental vibration-rotation band have been obtained with all the different experimental conditions described. They have been displayed and the spectral lines identified. For each branch of any band, at least one line is specified on each spectrum to be presented for orientation purposes.

3.1 LABORATORY STUDIES

3.1.1 High Temperature Emission Spectrum

A 0.2 cm^{-1} resolution emission spectrum of a Bernzomatic® torch is shown from 1, 800 to 3, 700 cm^{-1} in Fig. 4. The spectrum is dominated by the very strong CO_2 ν_3 fundamental band that swamps all other radiation from 2, 200 to 2, 400 cm^{-1} and has considerable intensity between 2, 100 and 2, 200 cm^{-1}. The CO_2 radiative structure at frequencies smaller than 2, 200 cm^{-1} is primarily attributable to hot lines ($v'v''$ = 2-1; 3-2; etc.) found at elevated temperatures characteristic of combustion gases. (The temperature at the center of a Bernzomatic torch flame is approximately 1, 500°K.) However, much CO structure can be seen riding on the CO_2 continuum in the 2, 100 to 2, 200 cm^{-1} region, and CO lines are the primary spectral features between 2, 000 and 2, 100 cm^{-1}. This survey spectrum immediately suggests that the R branch of the CO fundamental band, which lies

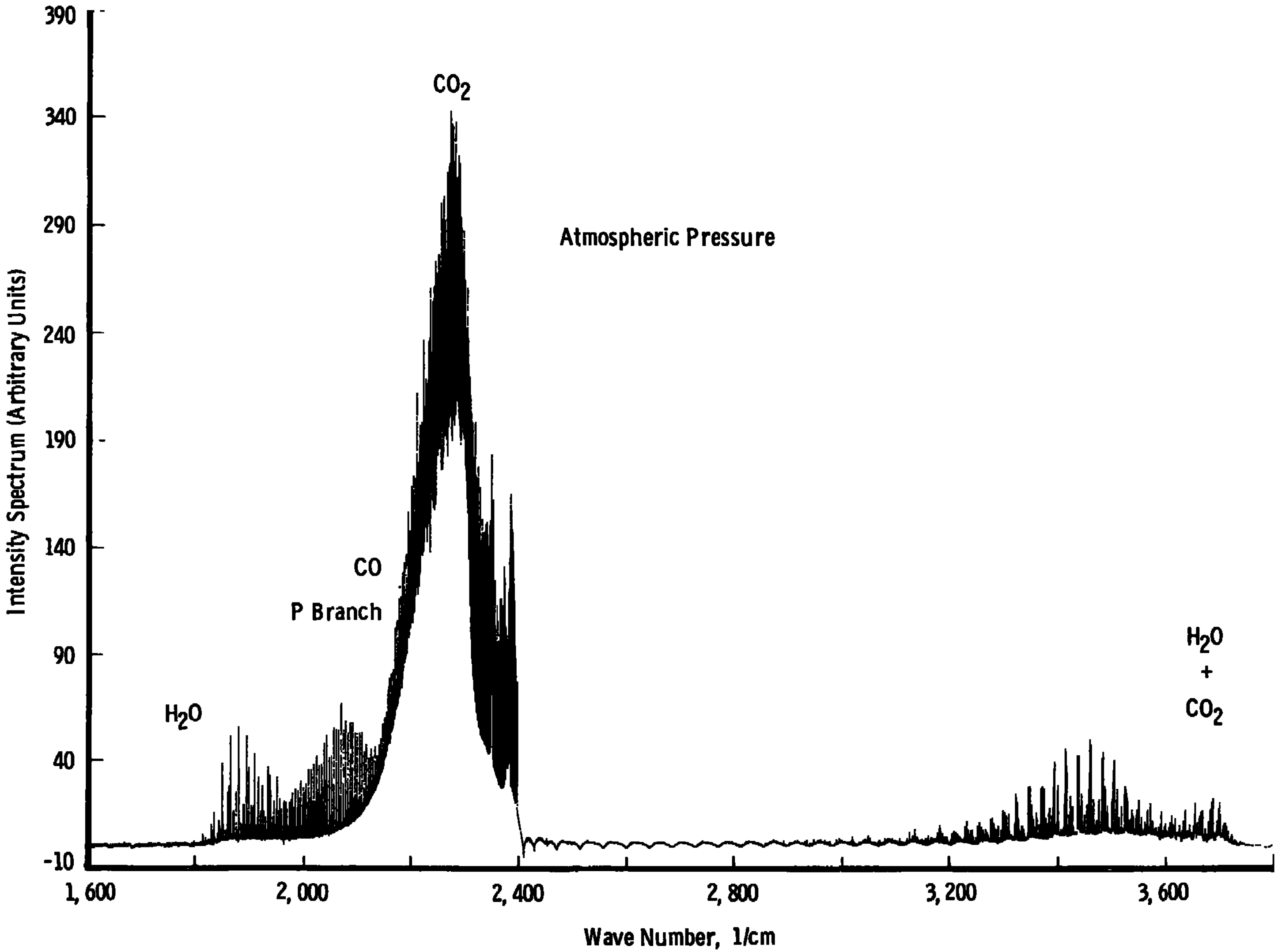

Figure 4. Emission spectrum of bernzomatic torch (1,800 to 3,700 cm^{-1}, 0.2 cm^{-1} resolution).

closest to the CO_2 ν_3 band is strongly overlapped by the hot CO_2 spectrum, but that the P branch suffers little CO_2 interference. The clear lines are most desirable for use in analysis, but the lines riding on the continuum can be useful where the continuum is not too strong. This is seen more clearly in Fig. 5, which is an expansion of the 2,000 to 2,200 cm^{-1} region of the Bernzomatic torch spectrum with CO and H_2O emission lines identified. The lower frequency lines in the CO P branch suffer progressively more frequent interference from H_2O lines of the H_2O ν_2 band centered at 1,595 cm^{-1}.

3.1.2 Moderate Temperature Absorption Cell Spectrum

Figure 6 shows an absorption spectrum of a 10-torr, room temperature sample of CO contained in a 10-cm-long, glass absorption cell with calcium fluoride windows at either end. The resolution in the spectrum is 0.07 cm^{-1}. The stability, low noise level, and high resolution derived from this operating procedure make weak lines more obvious than in the flame spectrum. In this spectrum, lines of the naturally occurring CO isotopes $C^{13}O^{16}$ and $C^{12}O^{18}$ are also clearly discernible. This spectrum reveals those $C^{12}O^{16}$ lines which are overlapped by isotopic CO lines and which are therefore not the most desirable for use in infrared analyses.

3.2 TEST CELL STUDIES

3.2.1 High Temperature Rocket Plume

Figure 7 is a spectrum of the 1,000-lbf thrust liquid propellant (N_2O_4/MMH) rocket plume taken during a firing in test cell T-3. The particular engine configuration in this case was the one listed in Table 1. The O/F ratio was 1.8, and the test cell was operated at a simulated altitude of 110,000 ft. The resolution in the spectrum of Fig. 7 is 0.3 cm^{-1}. A bandpass filter was used to isolate the 2,000 to 2,150 cm^{-1} region. This filter minimizes noise and interference due to the CO_2 ν_3 band and the H_2O ν_2 band, giving a clearer picture of the most useful spectral range for study of CO. Rocket performance properties for this measurement were calculated using the NASA rocket performance program (Ref. 4) and are shown in Table 2. This data suggests the nature of the sample involved. Calculations made with the Lockheed method of characteristics plume expansion computer program (Ref. 5) indicate that the plume temperature along the centerline decreased by about

130°K in the first three inches from the exit plane. The entire segment of the cell centerline within the field of view of the interferometer would then be above 1,000°K. The spectrum shows two regular series of lines representing the 1-0 and 2-1 CO bands, interspersed with scattered water vapor lines.

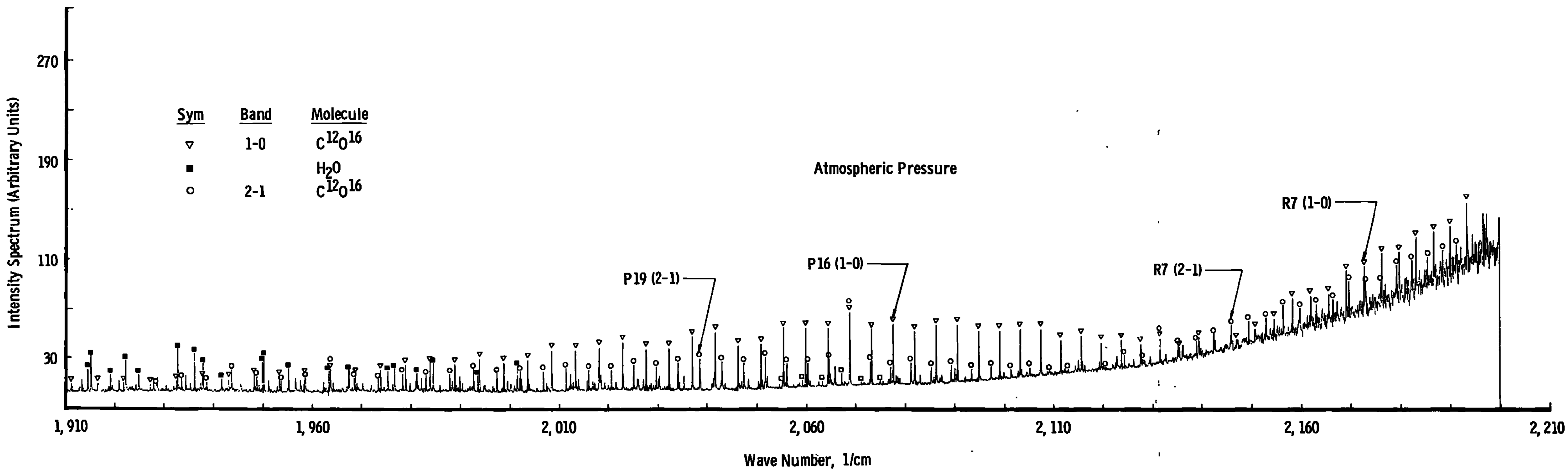

Figure 5. Emission spectrum of bernzomatic torch (1,900 to 2,200 cm^{-1}, 0.2 cm^{-1} resolution).

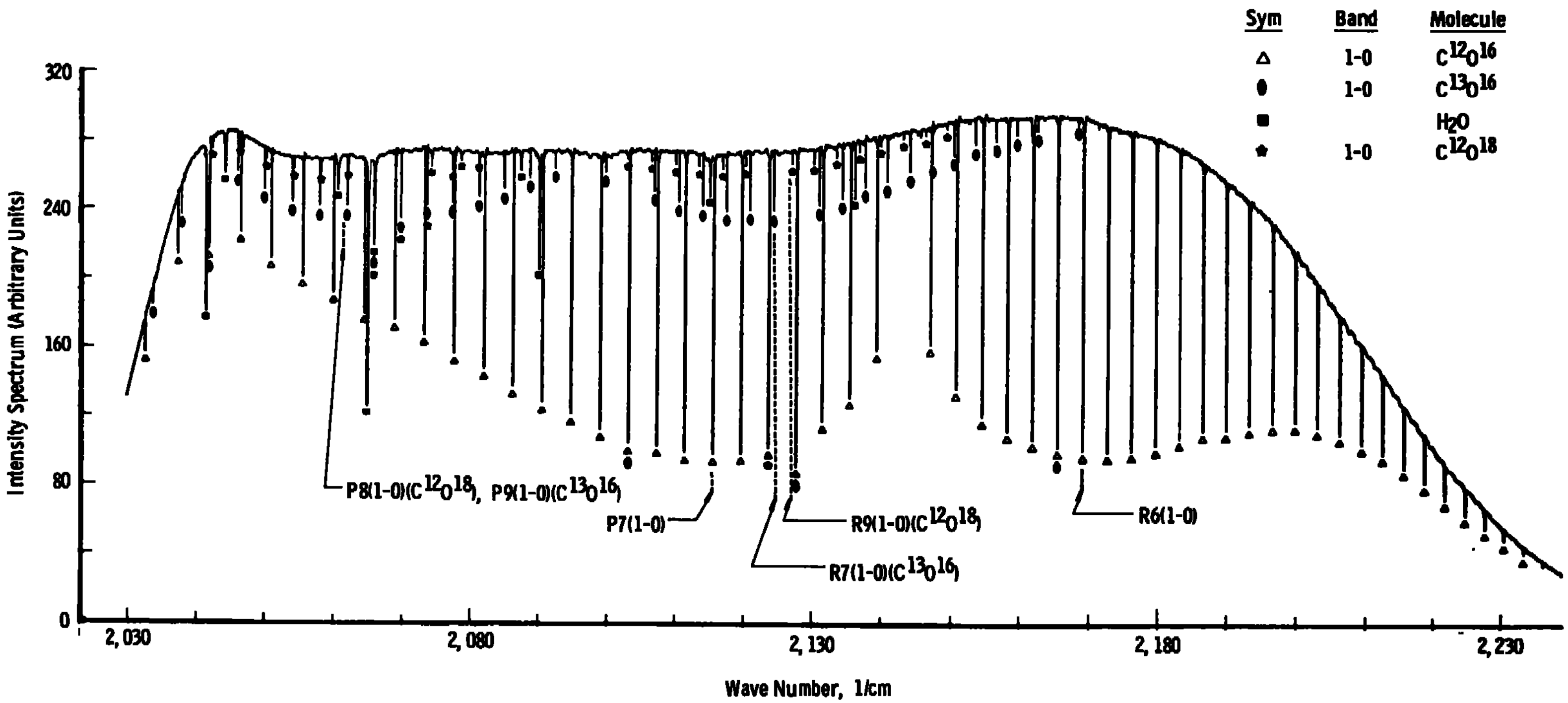

Figure 6. Absorption spectrum of CO at room temperature and a pressure of 10 torr (2,030 to 2,230 cm^{-1}, 0.07 cm^{-1} resolution).

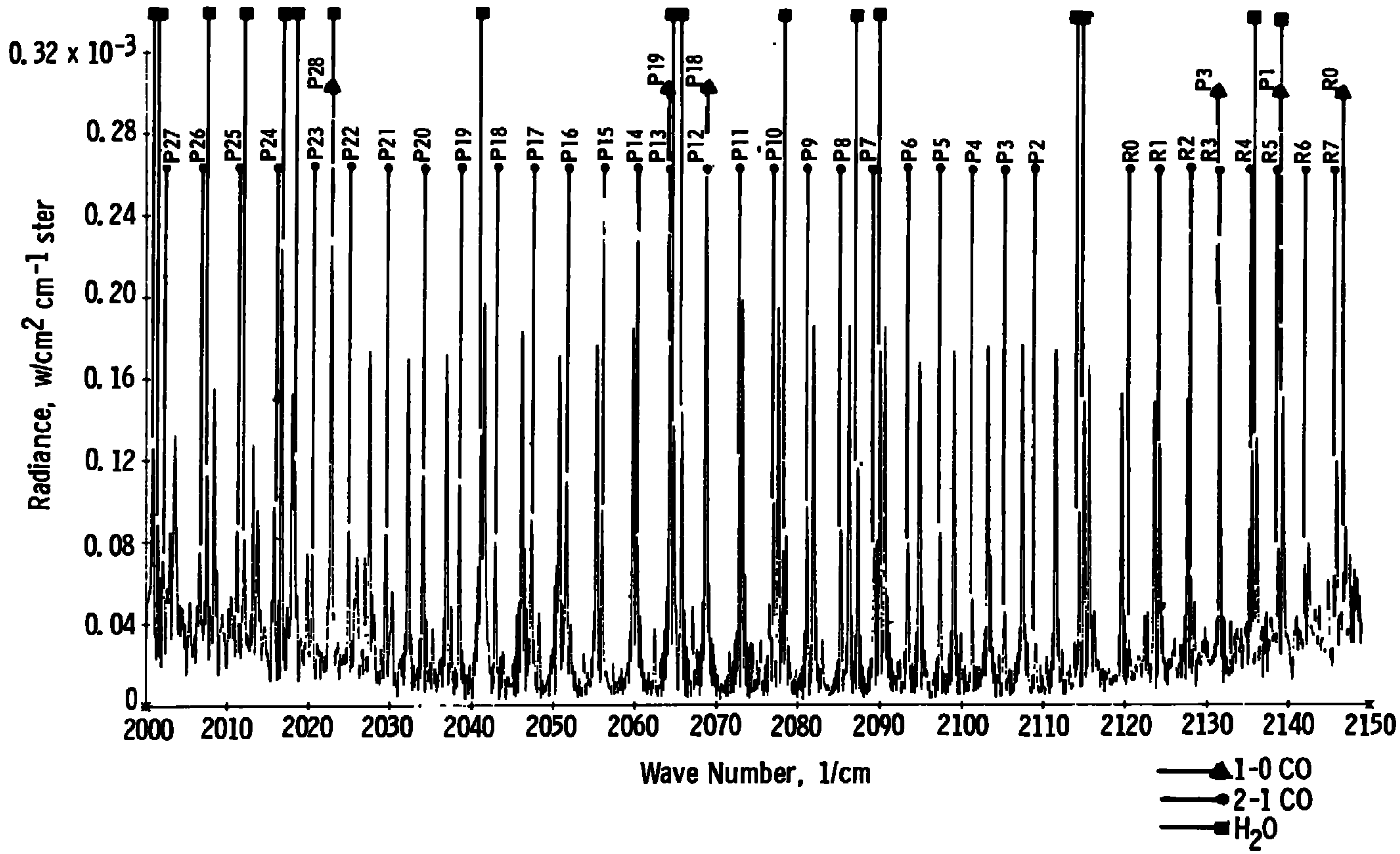

Figure 7. Emission spectrum of rocket plume in T-3 Test Cell (2,000 to 2,150 cm^{-1}, 0.3 cm^{-1} resolution).

Table 2. Theoretical Rocket Performance Assuming Equilibrium Composition During Expansion of a 1,000-lbf Thrust Rocket in Test Cell T-3

O/F = N_2O_4/MMH = 1.82

Equivalence Ratio = 1.3716

Cell Pressure = 5.3 torr (110,000 ft)

Chamber Pressure = 500 psia

	Exit Plane Conditions
Exit Static Pressure, atm	0.1189
Exit Static Temperature, °K	1,233
Density, gm/cc	2.5813×10^{-5}
Mach Number	4.0025
Nozzle Expansion Ratio (AE/AT)	25.0

Composition	Mole Fraction
CO	0.06891
CO_2	0.10026
H_2	0.16026
H_2O	0.34724
N_2	0.32333

3.2.2 Moderate Temperature Rocket Plume

A 0.3 cm^{-1} resolution emission spectrum of the 5-lbf thrust liquid propellant (N_2O_4/MMH) rocket plume in the R-2H test cell is shown from 2,000 to 2,450 cm^{-1} in Fig. 8. For this case a 5-lbf thrust, 40 to 1 nozzle expansion ratio, 1.6 O/F ratio engine configuration was used, and the test cell was operated at a simulated altitude of 225,000 ft.

The plume temperature in this case was lower than either the 1,000-lbf rocket plume or the Bernzomatic torch, which were discussed previously. The CO_2 ν_3 band in this case is confined to well resolved groups of lines between about 2,250 and 2,400 cm^{-1} and does not overlap the CO emission. In the CO fundamental, no hot lines are obvious, and the intensities of lines present are only a few

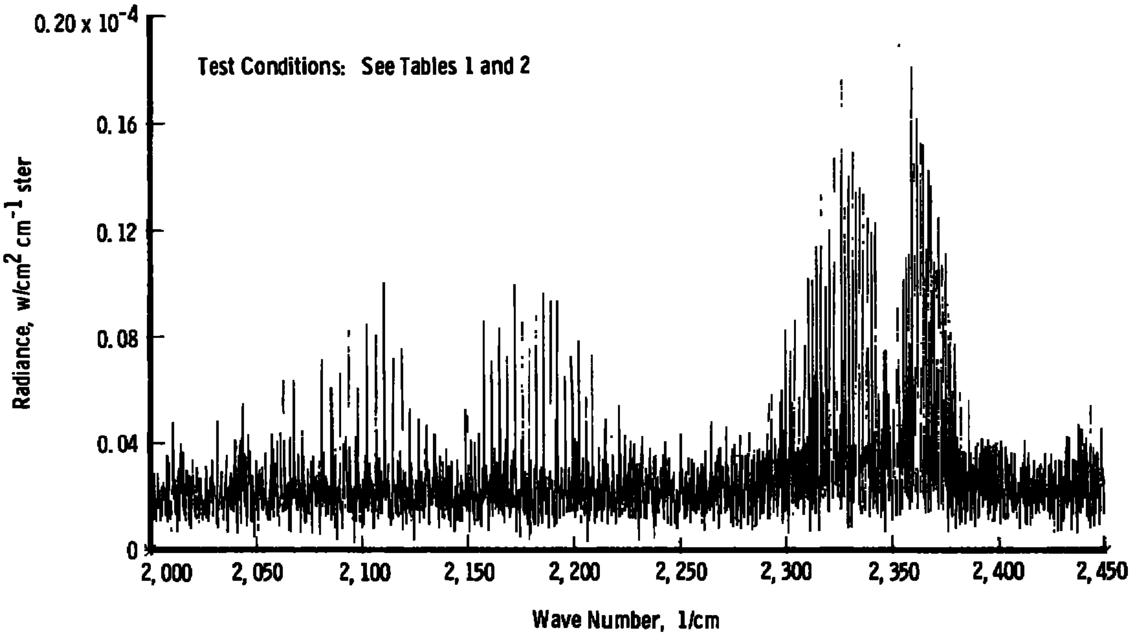

Figure 8. Emission spectrum of rocket plume in R-2H Test Cell (2,000 to 2,450 cm^{-1}, 0.3 cm^{-1} resolution).

percent of their counterparts in the spectrum for the 1,000-lbf thrust rocket plume in Test Cell T-3. The intensity difference was due in part to the fact that the ratio of field of view to plume size was much larger for the 5-lbf rocket plume than for the 1,000-lbf plume. Calculations (Ref. 5) indicate a plume temperature drop along the centerline of about 240°K within the field of view of the interferometer. An expanded plot of this CO spectrum is shown in Fig. 9, in which the lines are identified. Properties of the 5-lbf thrust rocket, calculated using Ref. 4, are shown in Table 3.

3.3 LINES FOR COMBUSTION GAS DIAGNOSTICS

Several isolated CO lines suitable for use in combustion gas diagnostics were found by observing the previously introduced spectra. Since the number and location of the isolated lines depend to some extent on the temperature of the source, three lists were prepared corresponding to high and moderate temperature samples and lines common to both samples. The lists are limited to lines which fell within the spectral range studied for each type of sample. Table 4 lists lines that are suitable for use with moderate temperature samples, and Table 5 gives similar information for high temperature samples (>1,000°K). Table 6 contains lines common to both Tables 4 and 5.

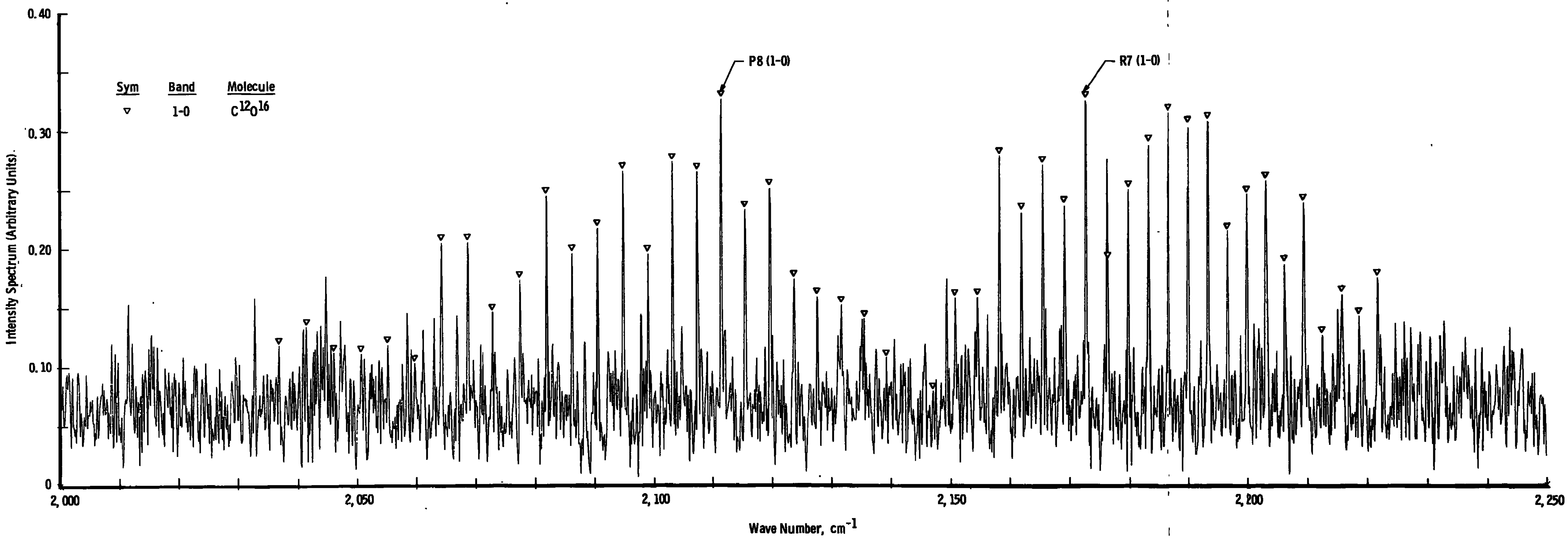

Figure 9. Emission spectrum of rocket plume in R-2H Test Cell (2,000 to 2,250 cm-1, 0.3 cm-1 resolution).

Table 3. Theoretical Rocket Performance Assuming Equilibrium Composition During Expansion of a 5-lbf Rocket in Test Cell R-2H

$O/F = N_2O_4/MMH = 1.59$

Equivalence Ratio = 1.57

Cell Pressure = 0.07 torr (225,000 ft)

Chamber Pressure = 50 psia

	Exit Plane Conditions
Exit Static Pressure, atm	0.0061
Exit Static Temperature, °K	952
Density, gm/cc	1.62×10^{-6}
Mach Number	4.45
Nozzle Expansion Ratio (AE/AT)	25.0

Composition	Mole Fraction
CO	0.06
CO_2	0.11
H_2	0.25
H_2O	0.26
N_2	0.31

Table 4. Isolated CO Lines in Moderate Temperature Samples

Line	Band	Wave Number, 1/cm
R22	(1-0)	2,221.75
R21		2,218.75
R20		2,215.70
R19		2,212.63
R18		2,209.51
R17		2,206.35
R15		2,199.93
R14		2,196.66
R12		2,190.02
R8		2,176.28
R6		2,169.20
R2		2,154.60
R1		2,150.86
P6		2,119.68
P8		2,111.54
P11		2,099.08
P12		2,094.86
P21		2,055.40
P22		2,050.85

Note: These data were derived from R-2H test results and room temperature absorption cell measurements.

Table 5. Isolated CO Lines in High Temperature Samples

Line	Band	Wave Number, 1/cm
R22	(1-0)	2, 221.75
R21		2, 218.75
R20		2, 215.70
R19		2, 212.63
R18		2, 209.51
R14		2, 196.68
R2		2, 154.60
P8		2, 111.54
R21	(2-1)	2, 191.49
R20		2, 188.49
R17		2, 179.24
R6		2, 142.47
P1		2, 112.98
P2		2, 109.14
P6		2, 093.41
P15		2, 056.05

Note: These data were derived from Bernzomatic torch and T-3 test results.

Table 6. CO Lines Isolated in Both Moderate and High Temperature Samples

Line	Band	Wave Number, 1/cm
R22	(1-0)	2,221.75
R21		2,218.75
R20		2,215.70
R19		2,212.63
R18		2,209.51
R14		2,196.66
R2		2,154.60
P8		2,111.54

4.0 SUMMARY

Several high resolution spectra of samples containing CO were obtained in order to determine isolated CO lines which would be useful in combustion gas diagnostics. The samples involved different temperatures and contained other constituents (CO_2 and H_2O, for example) usually present in typical combustion gases. Spectra were obtained under both laboratory and test cell conditions. Several CO lines were identified which were well enough isolated from other CO, CO_2, and H_2O lines to be useful in a combustion gas diagnostics program.

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